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Computing Regression Quantiles

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# Computing Regression Quantiles

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Key Words and Phrases: Linear Models, Robust Estimation, Regression Quantiles, Empirical Processes, Parametric Linear Programming.

## Language

Fortran 66

## Description and Purpose

Some slight modifications of the well-known Barrodale and Roberts (1974) algorithm for least absolute error estimation of the linear regression model are described. The modified algorithm computes the regression quantile statistics of Koenker and Bassett (1978) and the associated empirical quantile (and distribution) functions. These methods have applications to robust estimation and inference for the linear model.



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## Theory

The  $\ell_1$ -estimator in the linear model,

$$Y_i = x_i \beta + u_i, \quad u_i \sim iid F_u, \quad (1.1)$$

which solves over  $b \in \mathbb{R}^p$ ,

$$R(b) = \sum_{i=1}^n |y_i - x_i b| = \min! \quad (1.2)$$

provides a natural generalization of the sample median to the general linear regression model. This observation raises the question: Are there equally natural analogues of the rest of the sample quantiles for the linear model?

An affirmative answer is offered in Koenker and Bassett(1978) where  $p$ -dimensional "regression quantiles" are defined as solutions to

$$R_\theta(b) = \sum_{i=1}^n \rho_\theta(y_i - x_i b) = \min! \quad (1.3)$$

where  $\theta \in (0,1)$  and

$$\rho_\theta(u) = \begin{cases} \theta u & u \geq 0 \\ (\theta-1)u & u < 0 \end{cases}$$

In the one-sample (location) problem, solutions to (1.3) are simply the  $\theta^{th}$  sample quantiles from the sample  $(y_1, \dots, y_n)$ .

The asymptotic theory of the ordinary sample quantiles extends in a straightforward way to the joint asymptotic behavior of finitely many regression quantiles. See Koenker and Bassett(1978), Ruppert and Carroll(1980) and the recent work of Jureckova (1983). Thus, the theory of linear combinations of sample quantiles, or L-estimators, is available to construct robust estimators of linear models based upon regression quantiles. Perhaps more significantly, it is possible to construct trimmed least squares estimators for the linear model whose asymptotic behavior mimics the theory of the trimmed mean, see Ruupert and Carroll (1980). Recently, Jureckova (1983) has demonstrated the close connection between these trimmed least squares estimators and Huber's M-estimators for the linear model. Dejongh and DeWet(1984a,b) have also investigated this approach.

Estimates of the conditional quantile, and distribution, functions of  $Y$  given  $x$  may also be constructed based on these methods. For the model (1.1) we may define the conditional quantile function of  $Y$  at  $x$  as

$$Q_Y(\theta|x) = x \beta + F_u^{-1}(\theta)$$

And the conditional distribution function of  $Y$  is simply,

$$F_Y(Y|x) = \sup\{\theta | Q_Y(\theta|x) \leq y\}.$$

Clearly,  $F_Y(\cdot)$  is simply a translation of  $F_u(\cdot)$  under the iid error hypothesis.

Bassett and Koenker(1982) propose the estimate

$$\hat{Q}_Y(\theta) = \inf\{xb \mid R_\theta(b) = \min!\}.$$

For reasons developed there, interest focuses on  $\hat{Q}_Y$  at the mean of the design, that is, on  $\hat{Q}_Y(\theta) = \hat{Q}_Y(\theta|\bar{x})$ . The corresponding estimate of the conditional distribution function is simply,

$$\hat{F}_Y(y|x) = \sup\{\theta \mid \hat{Q}_Y(\theta|x) \leq y\}$$

and we will write  $\hat{F}_Y(y)$  for  $\hat{F}_Y(y|\bar{x})$ .

In Bassett and Koenker(1982) it is shown that  $\hat{Q}_Y(\cdot)$  is a proper quantile function -- a monotone jump function on the interval  $[0,1]$ , and under mild regularity conditions, that the random function,

$$Z_n(\theta) = \sqrt{n}(F_Y(\hat{Q}_Y(\theta)) - \theta)$$

has finite dimensional distributions which converge to those of the Brownian Bridge. Portnoy (1983) has recently shown that the process  $Z_n(\theta)$  is tight and consequently converges weakly to the Brownian Bridge.

Thus,  $\hat{F}_Y(\cdot)$  provides a reasonable alternative to estimates based on residuals (from some preliminary estimate of the vector  $\beta$ ) for diagnostic checking of distributional hypotheses and also perhaps for implementing recent proposals for bootstrapping and adaptive estimation of linear models which rely on estimates of the shape of the error distribution.

## Method

Barrodale and Roberts(1973) proposed a modified simplex algorithm for the  $\ell_1$ -estimation problem (1.1) which substantially improves upon earlier algorithms in speed and simplicity. Trivial modifications are required to adapt the Barrodale and Roberts algorithm to solve the "regression quantile" problem (1.3) for a fixed value of  $\theta$ . One simply adds the scalar THETA to the calling sequence, declares it real, and replaces the statement immediately preceding the statement labeled 50 with the statements:

WGT=SIGN(1.0,A(I,N2))

SUM=SUM + A(I,J)\*(2.0 \* THETA \* WGT + 1.0 - WGT)

However, to compute  $\hat{Q}_Y(\cdot)$  and  $\hat{F}_Y(\cdot)$  one must solve (1.3) for all values of  $\theta \in [0,1]$ . This is slightly more complex, requiring the solution to a *parametric* linear program. See Gal(1979) for comprehensive treatment of this general class of problems.

For any  $\theta_0 \in (0,1)$ , there exist solutions to the problem (1.3) of the form,

$$b_h = X_h^{-1}y_h \tag{2.1}$$

where the subscript  $h$  denotes a  $p$ -element subset of the first  $n$  integers,  $X_h$  is the  $p \times p$  submatrix of  $X$  consisting of the rows indexed by  $h$ , and  $y_h$  denotes the corresponding subvector of  $y$ . Indeed the set of the solutions to (1.3) is a polytope with extreme points of this form. In the terminology of linear programming  $b_h$  is a "basic" solution.

Such a solution is optimal at  $\theta_0$  if and only if, it satisfies the subgradient condition,

$$(\theta_0 - 1)\mathbf{1}_p \leq \sum_{i \in h} [u_i - sgn(y_i - x_i b_h) - \theta_0] x_i b_h \leq \theta_0 \mathbf{1}_p, \quad (2.2)$$

where  $\mathbf{1}_p$  denotes a  $p$ -vector of ones. Thus, for  $\theta \neq \theta_0$ ,  $b_h$  remains optimal until these  $p$  double inequalities are violated. So, starting from  $\theta_0$ , we have  $2p$  inequalities in  $\theta$

$$(0-1) \leq a_j + d_j \theta \leq \theta \quad j=1, \dots, p \quad (2.3)$$

with the  $a_j$ 's and  $d_j$ 's defined in the obvious way from (2.2). This decomposition of the "gradient" is stored in two new rows of the Barrodale and Roberts simplex tableau. To compute the next value of  $\theta$  i.e. the value of  $\theta$  at which  $b_h$  ceases to be optimal, we find

$$\theta_1 = \min_{\theta > \theta_0} \{a_j/(1-d_j), (a_j+1)/(1+d_j), \quad j=1, \dots, p\}. \quad (2.4)$$

At  $\theta_1$ , we make one simplex pivot from  $b_h$  to a new basic solution  $b_h'$ , which differs in only one element of  $h$ , recompute the  $a$ 's and  $d$ 's, and continue the iteration.

In practice we use instead,

$$\theta_1' = \theta_1 + (\epsilon + \epsilon/|1+d'|) ||X||$$

where  $\epsilon$  is a tolerance parameter specified below,  $d'$  is the value the  $d_j$  at which the minimum occurs in (2.4) and  $||X||$  is a norm of the design matrix. We use,

$$||X|| = \max_i \sum_{j=1}^p |x_{ij}|.$$

This insures a distinct new solution with  $h' \neq h$ . Also, the user may specify values  $\theta_0$  and  $\theta_L$  at which to begin and end the iterations. The natural choice here is  $\theta_0 = 1/n$  and  $\theta_L = 1-1/n$ . Koenker and Bassett (1978) note that the residuals  $u_i(b) = y_i - x_i b$  from any solution  $\hat{\beta}$ , to the problem (1.3) satisfy the inequalities,

$$N = \#\{i | u_i(\hat{\beta}) < 0\} \leq n\theta \leq \#\{i | u_i(\hat{\beta}) \leq 0\} = N + Z$$

Since  $N = 0$  at  $\theta = 0$ , and  $N = 1$  at the first jump, say  $\theta_1$ , it follows that  $\theta_1 \geq 1/n$ . Similarly, the last jump  $\theta_L \leq 1 - 1/n$ .

Our modified algorithm returns an array dimensioned  $k \times 2$  whose first column contains a vector of quantiles and whose second column contains the mass associated with each quantile. Of course in the one sample problem, with  $X = \mathbf{1}_n$ , the second column is simply an  $n$ -vector with  $i^{th}$  element  $i/n$ . However, in general the mass associated with the quantiles is variable. The storage allocation for this array is somewhat problematic. For problems of modest size, say  $p < 10$  and  $n < 500$  we have found  $2n < k < 3n$  an adequate rule-of-thumb. However, for larger problems  $k$  may increase quite rapidly. Indeed, it is known, see Murty(1983), that there are worst-case parametric linear programs for which  $p=n/2$  and  $k=2^p$ . Whether these examples can be adapted to the special structure of problem (1.3) is an open question, but their existence suggests that there may be no polynomial upper bound in  $p$  and  $n$  for  $k$ .

## Implementation

The principle modification of the Barrodale and Roberts routine is the addition of three new rows of the array  $A$  which contains the simplex tableau. The three new rows of the tableau contain the decomposition of the marginal cost row:  $a$ 's and  $b$ 's appear in  $A(M+2, \cdot)$  and  $A(M+3, \cdot)$  respectively, and the vector  $\bar{x}$  is stored in  $A(M+4, \cdot)$ . The only substantive change in the code is the addition of the section labeled "compute next theta". Further modifications along the lines suggested by Bloomfield and Steiger(1980) may improve the efficiency of the algorithm somewhat. The recent work of Karmarker(1984) may lead to further improvements especially for large problems. The tolerance parameter  $\epsilon$  referred to above is chosen to be the smallest safely detectable value of  $|x-y|/x$ , see for example the routine R1MACH in Fox(1976).

## Structure

CALL RQ(N,P,N5,P2,X,Y,T,TOLER,B,E,S,WX,WY,NSOL,SOLP,SOLQ,LSOL)

### Formal Parameters

N	Integer	Input:	Number of observations.
P	Integer	Input:	Number of parameters.
N5	Integer	Input:	N+5
P2	Integer	Input:	P+2
X	Real(N,P)	Input:	The problem design matrix.
Y	Real(N)	Input:	The response variable.
T	Real	Input:	The desired quantile. If T is not in [0,1], the problem is solved for all T in [0,1].
TOLER	Real	Input:	A small positive constant.
NSOL	Integer	Input:	Dimension of the solution array.
S	Integer(N)	Work:	
WX	Real(N5,P2)	Work:	
WY	Real(N)	Work:	
B	Real(P)	Output:	Optimal parameters at last t.
E	Real(N)	Output:	Optimal residuals at last t.
WX(N+1,P+1)		Output:	Objective function at last t.
WX(N+1,P+2)		Output:	Rank of design matrix.
WX(N+2,P+1)		Output:	Exit code: 0 = Solution nonunique. 1 = Solution OK.

$WX(N+2,P+2)$			<b>2</b> = Premature end.
$SOLP$	Real(NSOL)	Output:	<b>3</b> = $N5 \neq N+5$ .
$SOLQ$	Real(NSOL)	Output:	<b>4</b> = $P2 \neq P+2$ .
$LSOL$	Integer	Output:	Number of simplex iterations. A solution vector which contains the cumulative probability mass for each quantile.
			A solution vector of (monotone increasing) quantiles.
			Actual length of the solution vectors.

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## EXAMPLE: THE STACKLOSS DATA

```
PROGRAM MAIN
REAL X(21,3),WX(26,6),Y(21),WY(21),E(21),B(4),SOLP(42),SOLQ(42)
INTEGER S(21),LSOL
DATA TOLER/1.2E-7/
DO 1 I=1,21
X(I,1)=1.0
1 CONTINUE
READ (5,*) ((X(I,J),J=2,4),Y(I),I=1,21)
CALL RQ(21,4,26,6,X,Y,2.,TOLER,B,E,S,WX,WY,42,SOLP,SOLQ,LSOL)
WRITE(6,10)WX(23,5)
10 FORMAT("EXIT CODE=",F5.0)
WRITE(6,20)(SOLP(I),SOLQ(I),I=1,LSOL)
20 FORMAT(2F16.3)
STOP
END
```

### Stackloss Data

x1 x2 x3 y

80	27	89	42
80	27	88	37
75	25	90	37
62	24	87	28
62	22	87	18
62	23	87	18
62	24	93	19
62	24	93	20
58	23	87	15
58	18	80	14
58	18	89	14
58	17	88	13
58	18	82	11
58	19	93	12
50	18	89	8
50	18	86	7
50	19	72	8
50	19	79	8
50	20	80	9
56	20	82	15
70	20	91	15

Output from a VAX-11/780

exit code= 1.  
0.12411893 13.45404339  
0.13007915 13.99367046  
0.13038845 15.30951786  
0.14944933 15.30952358  
0.16074213 15.30952358  
0.22314128 15.30952072  
0.25399303 15.30952168  
0.27513024 15.30952549  
0.33102346 16.16141319  
0.37501332 16.44413567  
0.39190131 16.80134010  
0.40951341 16.95934868  
0.48986971 17.42450523  
0.56481242 17.43436623  
0.59239787 17.44517703  
0.00424811 17.45659256  
0.62001455 19.12624954  
0.65115529 19.13750839  
0.68975174 19.14842606  
0.76212549 19.15640259  
0.76345610 19.19264221  
0.77394605 19.71523857  
0.77770203 19.98903847  
0.81431276 20.12132454  
0.83394426 20.16070366  
0.91308522 20.20633698  
1.00000000 21.70072937

```

SUBROUTINE RQ(M,N,M5,N2,A,B,T,TOLER,X,E,S,WA,WB,NSOL,
*SOLP,SOLQ,LSOL)
DOUBLE PRECISION SUM
REAL MIN,MAX,A(M,N),X(N),WA(M5,N2),WB(M),E(M)
REAL B(M),SOLP(NSOL),SOLQ(NSOL)
INTEGER OUT, S(M)
LOGICAL STAGE, TEST,INIT,IEND
DATA BIG/1.E37/
C
C INITIALIZATION
C
M1 = M+1
N1 = N+1
M2 = M+2
M3 = M+3
M4 = M+4
DO 2 I=1,M
SUM = 0.0
WB(I)=B(I)
DO 1 J=1,N
WA(I,J)=A(I,J)
SUM = SUM + ABS(A(I,J))
1 CONTINUE
IF(SUM .GT. AMG)AMG = SUM
2 CONTINUE
IF(M5 .NE. M+5)WA(M2,N1) = 3.
IF(N2 .NE. N+2)WA(M2,N1) = 4.
IF(WA(M+2,N+1) .GT. 2.)RETURN
DIF = 0.0
IEND = .TRUE.
IF(T .GE. 0.0 .AND. T .LE. 1.0)GOTO 3
T0 = 1./FLOAT(M)-TOLER
T1 = 1. - T0
T = T0
IEND = .FALSE.
3 CONTINUE
INIT = .FALSE.
LSOL = 1
KOUNT = 0
DO 9 K=1,N
WA(M5,K) = 0.0
DO 8 I=1,M
WA(M5,K) = WA(M5,K) + WA(I,K)
8 CONTINUE
WA(M5,K) = WA(M5,K)/FLOAT(M)
9 CONTINUE
DO 10 J=1,N
WA(M4,J) = J
X(J) = 0.
10 CONTINUE
DO 40 I=1,M
WA(I,N2) = N+I
WA(I,N1) = WB(I)
IF(WB(I).GE.0.)GOTO 30
DO 20 J=1,N2
WA(I,J) = -WA(I,J)
20 CONTINUE
30 E(I) = 0.
40 CONTINUE
DO 42 J=1,N
WA(M2,J) = 0.0
WA(M3,J) = 0.0
DO 41 I=1,M
AUX = SIGN(1.0,WA(M4,J)) * WA(I,J)

```

```

        WA(M2,J) = WA(M2,J) + AUX * (1.0 - SIGN(1.0,WA(I,N2)))
        WA(M3,J) = WA(M3,J) + AUX * SIGN(1.0,WA(I,N2))
41    CONTINUE
        WA(M3,J) = 2.0 * WA(M3,J)
42    CONTINUE
        GO TO 48
43    CONTINUE
        LSOL = LSOL + 1
        DO 44 I=1,M
        S(I) = 0.0
44    CONTINUE
        DO 45 J=1,N
        X(J) = 0.0
45    CONTINUE
C
C COMPUTE NEXT T
C
        SMAX = 2.0
        DO 47 J=1,N
        B1 = WA(M3,J)
        A1 = (-2.00 - WA(M2,J))/B1
        B1 = -WA(M2,J)/B1
        IF(A1 .LT. T)GO TO 46
        IF(A1 .GE. SMAX) GO TO 46
        SMAX = A1
        DIF = (B1 - A1 )/2.00
46    IF(B1 .LE. T) GO TO 47
        IF(B1 .GE. SMAX)GO TO 47
        SMAX = B1
        DIF = (B1 - A1)/2.00
47    CONTINUE
        TNT = SMAX + TOLER * (1.00 + ABS(DIF)) * AMG
        IF(TNT .GE. T1 + TOLER)IEND = .TRUE.
        T = TNT
        IF(IEND)T = T1
48    CONTINUE
C
C COMPUTE NEW MARGINAL COSTS
C
        DO 49 J=1,N
        WA(M1,J) = WA(M2,J) + WA(M3,J) * T
49    CONTINUE
        IF(INIT) GO TO 265
C
C STAGE 1
C
C DETERMINE THE VECTOR TO ENTER THE BASIS
C
        STAGE=.TRUE.
        KR=1
        KL=1
70    MAX=-1.
        DO 80 J=KR,N
        IF(ABS(WA(M4,J)).GT.N)GOTO 80
        D=ABS(WA(M1,J))
        IF(D.LE.MAX)GOTO 80
        MAX=D
        IN=J
80    CONTINUE
        IF(WA(M1,IN).GE.0.)GOTO 100
        DO 90 I=1,M4
        WA(LIN)=-WA(I,IN)
90    CONTINUE
C

```

```

C DETERMINE THE VECTOR TO LEAVE THE BASIS
C
100 K=0
    DO 110 I=KL,M
    D=WA(I,IN)
    IF(D.LE.TOLER)GOTO 110
    K=K+1
    WB(K)=WA(I,N1)/D
    S(K)=I
    TEST=.TRUE.
110 CONTINUE
120 IF(K.GT.0)GOTO 130
    TEST=.FALSE.
    GOTO 150
130 MIN=BIG
    DO 140 I=1,K
    IF(WB(I).GE.MIN)GOTO 140
    J=I
    MIN=WB(I)
    OUT=S(I)
140 CONTINUE
    WB(J)=WB(K)
    S(J)=S(K)
    K=K-1
C
C CHECK FOR LINEAR DEPENDENCE IN STAGE 1
C
150 IF(TEST.OR..NOT.STAGE)GOTO 170
    DO 160 I=1,M4
    D=WA(I,KR)
    WA(I,KR)=WA(I,IN)
    WA(I,IN)=D
160 CONTINUE
    KR=KR+1
    GOTO 260
170 IF(TEST)GOTO 180
    WA(M2,N1)=2.
    GOTO 390
180 PIVOT=WA(OUT,IN)
    IF(WA(M1,IN)-PIVOT-PIVOT.LE.TOLER)GOTO 200
    DO 190 J=KR,N1
    D=WA(OUT,J)
    WA(M1,J)=WA(M1,J)-D-D
    WA(M2,J)=WA(M2,J)-D-D
    WA(OUT,J)=-D
190 CONTINUE
    WA(OUT,N2)=-WA(OUT,N2)
    GOTO 120
C
C PIVOT ON WA(OUT,IN)
C
200 DO 210 J=KR,N1
    IF(J.EQ.IN)GOTO 210
    WA(OUT,J)=WA(OUT,J)/PIVOT
210 CONTINUE
    DO 230 I=1,M3
    IF(I.EQ.OUT)GOTO 230
    D=WA(I,IN)
    DO 220 J=KR,N1
    IF(J.EQ.IN)GOTO 220
    WA(I,J)=WA(I,J)-D*WA(OUT,J)
220 CONTINUE
230 CONTINUE
    DO 240 I=1,M3

```

```

IF(I.EQ.OUT)GOTO 240
WA(L,IN)=-WA(L,IN)/PIVOT
240 CONTINUE
    WA(OUT,IN)=1./PIVOT
    D=WA(OUT,N2)
    WA(OUT,N2)=WA(M4,IN)
    WA(M4,IN)=D
    KOUNT=KOUNT+1
    IF(.NOT.STAGE)GOTO 270
C
C INTERCHANGE ROWS IN STAGE 1
C
    KL=KL+1
    DO 250 J=KR,N2
        D=WA(OUT,J)
        WA(OUT,J)=WA(KOUNT,J)
        WA(KOUNT,J)=D
250 CONTINUE
260 IF(KOUNT+KR.NE.N1)GOTO 70
C
C STAGE 2
C
265 STAGE=.FALSE.
C
C DETERMINE THE VECTOR TO ENTER THE BASIS
C
270 MAX=-BIG
    DO 290 J=KR,N
        D=WA(M1,J)
        IF(D.GE.0.)GOTO 280
        IF(D.GT.(-2.))GOTO 290
        D=-D-2.
280 IF(D.LE.MAX)GOTO 290
    MAX=D
    IN=J
290 CONTINUE
    IF(MAX.LE.TOLER)GOTO 310
    IF(WA(M1,IN).GT.0.)GOTO 100
    DO 300 I=1,M4
        WA(I,IN)=-WA(I,IN)
300 CONTINUE
    WA(M1,IN)=WA(M1,IN)-2.
    WA(M2,IN)=WA(M2,IN)-2.
    GOTO 100
C
C COMPUTE QUANTILES
C
310 CONTINUE
    DO 320 I=1,KL-1
        K=WA(I,N2)*SIGN(1.0,WA(I,N2))
        X(K) = WA(I,N1) * SIGN(1.0,WA(I,N2))
320 CONTINUE
    SUM=0.0
    DO 330 I=1,N
        SUM=SUM + X(I) * WA(M5,I)
330 CONTINUE
    SOLP(LSOL) = T
    SOLO(LSOL) = SUM
    IF(IEND)GO TO 340
    INIT = .TRUE.
    GO TO 43
340 CONTINUE
    DO 350 I = 2,LSOL
        SOLP(I-1)=SOLP(I)

```

```
350 CONTINUE
      LSOL=LSOL-1
      SOLP(LSOL)=1.
      L =KL-1
      DO 370 I=1,L
      IF(WA(I,N1).GE.0.)GOTO 370
      DO 360 J=KR,N2
      WA(I,J)=-WA(I,J)
360 CONTINUE
370 CONTINUE
      WA(M2,N1)=0.
      IF(KR.NE.1)GOTO 390
      DO 380 J=1,N
      D=ABS(WA(M1,J))
      IF(D.LE.TOLER.OR.2.-D.LE.TOLER)GOTO 390
380 CONTINUE
      WA(M2,N1)=1.
390 DO 400 I=KL,M
      K = WA(I,N2) * SIGN(1.0,WA(I,N2))
      D = WA(I,N1) * SIGN(1.0,WA(I,N2))
      K=K-N
      E(K)=D
400 CONTINUE
      WA(M2,N2)=KOUNT
      WA(M1,N2)=N1-KR
      SUM = 0.0
      DO 410 I=1,M
      SUM = SUM + E(I)*(5. + SIGN(1.0,E(I))*(T-.5))
410 CONTINUE
      WA(M1,N1) = SUM
      RETURN
      END
```



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